

Protection of quantum systems by nested dynamical decoupling

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Based on a theorem we establish on dynamical decoupling of time-dependent systems, we present a scheme of nested Uhrig dynamical decoupling (NUDD) to protect multi-qubit systems in generic quantum baths to arbitrary decoupling orders, using only single-qubit operations. The number of control pulses in NUDD increases polynomially with the decoupling order. For general multi-level systems, this scheme can preserve a set of unitary Hermitian system operators which mutually either commute or anti-commute, and hence all operators in the Lie algebra generated from this set of operators, generating an effective symmetry group for the system up to a given order of precision. NUDD can be implemented with pulses of finite amplitude, up to an error in the second order of the pulse durations.

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I. INTRODUCTION

Both in high-precision magnetic resonance spectroscopy and in quantum computing, it is essential to suppress unwanted couplings within a quantum system and between the system and its environment (or bath). Such couplings result in population relaxation, phase randomization (pure dephasing), and more generally, unwanted evolution of certain system operators. Dynamical decoupling (DD) is a so-called open-loop control scheme to average out the system-bath interactions through stroboscopic operations of the system (without direct control on the environment). DD originated from the Hahn echo [1] and has evolved into variations with complicated sequences [2] for high-precision [3, 4] and multi-dimensional [5] magnetic resonance spectroscopy. When the field of quantum computing was opened up, DD was introduced to protect qubit coherence [6, 7]. By unitary symmetrization procedure [8, 9], DD cancels errors of quantum evolutions up to the first order in the Magnus expansion, and the corresponding cyclic scheme is referred to as periodic DD. A geometric understanding of the symmetrization procedure was given in Ref. [10]. To eliminate errors to the second order in the Magnus expansion, mirror-symmetric arrangement of two DD sequences (SDD) can be used [9]. A particularly interesting scheme is the concatenated DD (CDD) [11–14], which uses recursively constructed pulse sequences to eliminate decoherence to an arbitrary decoupling order (defined as the power of the total evolution time, which is assumed short). The performance of CDD was experimentally demonstrated for spins in solid-state environments [15]. The number of pulses used in CDD, however, increases exponentially with the decoupling order. Since errors are inevitably introduced in each control pulse in experiments, finding DD schemes with fewer control pulses is desirable.

For suppressing pure dephasing of single qubits (two-level systems) subjected to unidirectional noises, a remarkable advance is the optimal DD discovered by Uhrig [16] in a spin-boson model. Uhrig DD (UDD) is optimal in the sense that the

number of control pulses is minimum for a given decoupling order. It was later conjectured [17, 18] and then rigorously proven [19] that UDD is model-independent for any two-level systems coupled to a finite quantum bath. It was shown that UDD also works for suppressing longitudinal relaxation [19]. The ideal δ -pulses assumed in DD can be generalized to include some components of finite amplitude [19]. Recently, a method to incorporate shaped pulses of finite amplitude into UDD paves the way of realistic experiments [20]. UDD was first verified in experiments by microwave control of trapped ions in various artificial classical noises [21–23], and then UDD against realistic quantum noises was realized for radical electron spins in irradiated malonic acid crystals [24].

For suppressing the general decoherence of single qubits (including both pure dephasing and longitudinal relaxation), the concatenation of UDD sequences (CUDD) was proposed to reduce the number of control pulses [25]. For suppressing the decoherence up to an order N , the number of pulses required in CUDD is $\sim (N+1)2^N$, which is considerably less than $\sim 4^N$ as in CDD. Recently, West *et al* proposed a much more efficient scheme, called quadratic DD (QDD), to combat general decoherence of a qubit [26]. QDD is constructed by nesting two levels of UDD sequences, using $(N+1)^2$ control intervals to achieve the N th decoupling order. Numerical search indicates that QDD is near-optimal as it differs from the optimal solutions by no more than two pulses for a small decoupling order ($N \leq 4$) [26]. The validity of UDD can be extended to analytically time-dependent Hamiltonians [27]. This extension seems to validate QDD since the UDD sequence on the outer level can be viewed as acting on a time-dependent Hamiltonian resulting from the UDD control on the inner level. However, as we will show in Sec. III, the effective Hamiltonian resulting from the inner UDD sequences is only piecewise analytic in time, and actually there are counter examples in which UDD on the outer level does not achieve the designed decoupling order if the order of UDD on the inner level is *odd* and *lower* than the order of the outer UDD. Thus it remains an open question why QDD works. In the attempt to prove the validity of QDD, we establish a theorem: UDD applies to time-dependent Hamiltonians, regardless of their analytic properties, as long as the Hamiltonians between two adjacent pulses of the UDD sequence are symmetric and have the same function form of relative time between the ad-

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jacent pulses (see Sec. IID). Therefore we give a proof of the validity of QDD with even order UDD on the inner level. We note that the validation of QDD is still incomplete since the theorem mentioned above does not apply to QDD with odd order UDD on the inner level.

So far, the research of optimal DD focuses on the single-qubit decoherence problem, with some attempts on optimal DD to multi-level systems with prior knowledge of the initial states [28, 29]. For practical large-scale quantum computing, the issue is the decoherence, or more generally, the decay of quantum correlations (such as entanglement) of coupled multi-qubit systems. Therefore it is highly desirable to have a general arbitrary-order DD scheme for multi-qubit systems, with the number of pulses as small as possible. In addition, the DD scheme should preferably involve relatively easy implementations, for example, single-qubit operations. Realizations of the symmetrization procedure [8, 9] by averaging over so-called *nice* error bases [30] are explicitly given in Ref. [31]. However, each control operation in general is complicated and may involve manipulation on all qubits for multi-qubit systems. It would be of practical interest if there is an explicit, systematic, and efficient way to protect a particular set of operators of a quantum system to an arbitrary order.

In this paper, we give systematic and explicit DD schemes to protect multi-qubit systems arbitrarily coupled to quantum baths. The schemes are realized by protecting a set of mutually commuting or anti-commuting unitary Hermitian system operators on different levels. We call it a mutually orthogonal operation set (MOOS) in this paper. For example, the Pauli operators of qubits form an MOOS. The inner levels of DD control of operators in an MOOS are not affected by the outer levels of DD control. Furthermore, based on the above-mentioned theorem on DD of time-dependent systems, higher order protection of an MOOS can be achieved by nesting even-order UDD sequences on different levels. If a set of system operators is protected by such nested UDD (NUDD), then all system operators in the Lie algebra generated from this set of operators are protected to the same decoupling order, which indeed generates an effective symmetry group [8] of the system up to an error of the decoupling order. For multi-qubit systems, each control operation in DD only involves single-qubit manipulation. In addition, we will show that NUDD can be implemented with pulses of finite amplitude, which approximate ideal δ -pulses up to an error in the second order of the pulse durations, with the same pulse shaping as in Ref. [32]. For a general multi-level quantum system, we can also construct an MOOS and use NUDD to generate an effective symmetry group to a given decoupling order. It can be shown, however, that for a general M -level system, there may exist no MOOS to generate the whole basis of $\mathfrak{su}(M)$ algebra and hence the whole $SU(M)$ symmetry group. Further research is still needed to design efficient DD schemes (as compared with CDD) to protect general multi-level systems to higher orders.

This paper is organized as follows. In Sec. II, we present a general theory on protection of an MOOS by DD; NUDD is given based on a theorem established for UDD on time-

dependent systems. In this Section, the pulses in DD are assumed instantaneous. In Sec. III, we discuss NUDD on multi-qubit systems. In Sec. IV, we discuss DD with finite-amplitude pulses. Finally, we draw the conclusions in Sec. V.

II. PROTECTION OF SYSTEM OPERATORS

A. General formalism: MOOS

We consider a quantum system coupled to a general finite quantum bath, with a time-independent Hamiltonian

$$H = H_S + H_B + H_{SB}, \quad (1)$$

where H_S is the system Hamiltonian, H_B the bath one, and H_{SB} the system-bath interaction. We aim to find a sequence of stroboscopic operations O_1, O_2, \dots, O_q at times T_1, T_2, \dots, T_q in increasing order so that after the controlled evolution from $t = 0$ to $t = T$, a set of system operators

$$\{Q_j\} \equiv \{Q_1, Q_2, \dots\},$$

are conserved up to an error of $O(T^{N+1})$, i.e., for $(\hbar = 1)$

$$U \equiv e^{-iH(T-T_q)} O_q \dots O_2 e^{-iH(T_2-T_1)} O_1 e^{-iHT_1}, \quad (2)$$

we have

$$U^\dagger Q_j U = Q_j + O(T^{N+1}). \quad (3)$$

In this paper we assume that the bath is bounded in spectrum so that the perturbation expansion of U in a short time T is possible. To make DD efficient, it is required that the evolution of the system induced by the decoupling field be faster than the unwanted dynamics [6]. Here we assume that the control pulses are instantaneous and arbitrarily strong. Using pulses of finite duration and finite amplitude will be discussed in Sec. IV. Preferably, for a multi-qubit system, the operations O_j should contain only single-qubit operations. We also wish to use as few as possible operations to achieve a given order (N) of decoupling precision.

We note that when a set of operators $\{Q_j\}$ is preserved to a certain decoupling order, then all operators obtained by commutation $i[Q_j, Q_k]$, anti-commutation $[Q_j, Q_k]_+ \equiv Q_j Q_k + Q_k Q_j$, linear combinations, and their repetitions are also protected to the same decoupling order. All these protected operators form a Lie algebra, since they form a linear vector space and are close under the commutation operation. The Lie algebra defines a dynamically generated effective symmetry group S_Q of the system up to the decoupling order.

In particular, let us consider the protection of a set of operators $\{\Omega_j\}$ in which each pair of elements either commutes or anti-commutes. In our schemes, it is required that the operators $\{\Omega_j\}$ be unitary and satisfy $\Omega_j^2 = \pm 1$. Thus we choose Ω_j to be unitary and Hermitian, i.e.,

$$\Omega_j^2 = \Omega_j^\dagger \Omega_j = 1. \quad (4)$$

Note that Ω_j is a parity kick operator described in Ref. [33]. We will use the unitary Hermitian property of Ω_j to construct DD for protection of Ω_j .

Definition 1. An MOOS is defined as a set of operators which are unitary and Hermitian and have the property that each pair of elements either commutes or anti-commutes.

The commutation property of operators in an MOOS is important for constructing higher-order DD schemes, via the following theorem.

Theorem 1. For two operators Ω_1 and Ω_2 either commuting or anti-commuting with each other, if a unitary evolution $U(T)$ during a short time T commutes with Ω_1 up to an error of $O(T^{N+1})$, then $\Omega_2 U(T) \Omega_2$ also commutes with Ω_1 up to an error of $O(T^{N+1})$.

Proof. We directly calculate the commutator

$$[\Omega_1, \Omega_2 U(T) \Omega_2] = (-1)^\eta \Omega_2 [\Omega_1, U(T)] \Omega_2 = O(T^{N+1}),$$

where $\eta = +1$ (-1) for Ω_1 commuting (anti-commuting) with Ω_2 . \square

With this theorem, certain DD sequences protecting a given operator in an MOOS can be used as units to construct an outer level of DD protection of another operator in the MOOS, without affecting the DD effect of the inner level control. For operators which do not form an MOOS, the outer level control in general may interfere with the inner level control. For example, let us consider $\Omega_1 = \sigma_x$ and $\Omega_2 = (\sigma_x + \sigma_y) / \sqrt{2}$ (the Pauli matrix along the direction equally dividing the angle between the x - and y - axes). Suppose a DD sequence protects σ_x as $U(T) = e^{-i\sigma_x T + O(T^{N+1})}$. Then we apply a Hahn echo to protect Ω_2 , by the following evolution

$$U_2(2T) = \Omega_2 U(T) \Omega_2 U(T) = e^{-i\sigma_y T + O(T^{N+1})} e^{-i\sigma_x T + O(T^{N+1})}.$$

After the control on the outer level, the evolution actually does not commute with σ_x even in the leading order of T .

As we will show in Sec. II B, applying an element of an MOOS corresponds to a symmetrization procedure [8, 9] on one level, and protecting an MOOS will iteratively symmetrize the system evolution. An MOOS itself does not form a group or an algebra. However, it can generate a certain Lie algebra by commutation, anti-commutation, linear combinations, and repetitions. Therefore the protection of all operators in this Lie algebra is realized by the protection of this MOOS. For example, in a single-qubit system, N pulses of π -rotation control of the qubit about the z -axis, when arranged according to the UDD timing, protect the Pauli matrix σ_z and dynamically generate the symmetry group $SO(2)$ or $U(1)$, up to an error of $O(T^{N+1})$ [19]. For a pure dephasing Hamiltonian, which has $U(1)$ as its intrinsic symmetry group, the system under the UDD protection has the full $SU(2)$ symmetry. Another example is the N th order QDD sequence [26] consisting of pulses of σ_x and σ_y , which protects σ_x and σ_y and hence all operators in the $su(2)$ algebra (including σ_z), and therefore the qubit has a dynamically generated symmetry group $SU(2)$, up to an error of $O(T^{N+1})$.

Below we explicitly construct the MOOS for some particular Lie algebra to be protected:

1. For suppressing longitudinal relaxation of a single-qubit system along the z -direction, the MOOS contains only one operator σ_z .
2. For a general single-qubit system, two anti-commuting Pauli matrices, e.g., $\{\sigma_x, \sigma_y\}$, form an MOOS to protect all system operators [34].
3. For an L -qubit pure dephasing model in which H contains only the Pauli matrices along the z -direction, a choice of the MOOS is

$$\{\sigma_x^{(l)}\}_{l=1}^L \equiv \{\sigma_x^{(1)}, \sigma_x^{(2)}, \dots, \sigma_x^{(L)}\}.$$

Note that only single-qubit operators are used. It is obvious that all the Pauli matrices in the set commute with each other. There are totally L operators in the MOOS, which can be shown to be the minimum possible number.

4. For a general L -qubit system, to protect all operators of the system, i.e., the algebra $su(2^L)$, a choice of the MOOS is $\{\sigma_z^{(l)}, \sigma_x^{(l)}\}_{l=1}^L$. It is obvious that all the Pauli matrices either commute or anti-commute with each other. Note that only single-qubit operators are used. There are totally $2L$ operators in the MOOS, which can be shown to be the minimum possible number.
5. For a general M -level system, let us consider protection of all system operators which are diagonal in a certain orthonormal basis $\{|m\rangle\}_{m=0}^{M-1}$. Suppose $2^{L-1} < M \leq 2^L$. We can denote an integer number $0 \leq m < M$ using a binary code as $m = (m_L \dots m_2 m_1)$ with $m_l = 0$ or 1 . We define a unitary Hermitian operator

$$\Sigma_z^{(l)} = I - 2 \sum_{m_l=1} |m\rangle\langle m|. \quad (5)$$

A diagonal operator of the form $|m\rangle\langle m|$ can be written in terms of $\{\Sigma_z^{(l)}\}$ as

$$|m\rangle\langle m| = \prod_{l=1}^L \frac{I + (-1)^{m_l} \Sigma_z^{(l)}}{2}.$$

Thus any diagonal operators can be constructed using $\{\Sigma_z^{(l)}\}$. Actually, by adding $(2^L - M)$ ancillary basis states $\{|m\rangle\}_{m=M}^{2^L-1}$, the above-defined operators can be viewed as the single-qubit Pauli matrices along the z -direction ($\{\sigma_z^{(l)}\}$) of an L -qubit system projected to the M -level subsystem. It is obvious that all operators in $\{\Sigma_z^{(l)}\}$ commute with each other. Thus an MOOS is constructed. There are totally L such operators in the MOOS. Since an $(L-1)$ -qubit system has at least $(L-1)$ operators in an MOOS and $2^{L-1} < M \leq 2^L$, the MOOS $\{\Sigma_z^{(l)}\}_{l=1}^L$ contains the minimum number of operators (otherwise, we can construct a DD with less than M intervals to protect the system to the first decoupling order, which is impossible according to Ref. [31]).

6. For a given l , if $M/2^l$ is an integer, we can define unitary Hermitian operators anti-commuting with $\Sigma_z^{(l)}$ as

$$\Sigma_x^{(l)} = \sum_{m_l=0} \left(|m + 2^{l-1}\rangle \langle m| + \text{h.c.} \right), \quad (6)$$

which exchanges two basis states $|m\rangle$ and $|m'\rangle$ if m and m' differ at and only at the l th bit. Actually, the operator $\Sigma_x^{(l)}$ can be viewed as the Pauli matrix $\sigma_x^{(l)}$ of the l th qubit for a multi-qubit system. $\{\Sigma_x^{(l)} | M \bmod 2^l = 0\} \cup \{\Sigma_z^{(l)} | 2^l \leq M\}$ forms an MOOS of the M -level system.

Note 1: The choice of an MOOS for a certain system is not unique. For example, in the MOOS for generating $\text{su}(2^L)$ of a general L -qubit system, the two Pauli matrices $\sigma_z^{(l)}$ and $\sigma_x^{(l)}$ can be replaced with any two anti-commuting Pauli matrices of the l th qubit.

Note 2: For a general M -level system, there may exist no MOOS to generate the whole $\text{su}(M)$ algebra. For example, for an M -level system with M being an odd number, all operators in an MOOS must mutually commute and therefore are all diagonal in a common basis. This MOOS of course cannot generate the whole $\text{su}(M)$. Actually, if two operators Ω and Ω' in an MOOS anti-commute, we have $\text{Tr}(\Omega + \Omega'\Omega\Omega') = 2\text{Tr}(\Omega) = 0$, which is impossible for odd M .

For a general M -level system, the explicit operations given in Eqs. (5) and (6) are in general difficult to implement in experiments. It is important to find a suitable set of operations for a given multi-level system. It should also be noted that above we have assumed that all the operators in an MOOS are protected to the same decoupling order. In the CDD and NUDD schemes we will discuss later, different operators actually can be protected to different orders. In those cases, the precision of protection of the whole Lie algebra is determined by the lowest decoupling order.

B. Lowest order protection of system operators

A general DD framework to protect a set of operators to the lowest order is the symmetrization procedure over an appropriate DD group [8, 9]. Here we systematically give an explicit scheme to protect system operators forming an MOOS, which facilitates the construction of higher order DD in the later part of this paper.

Let us consider first protection of a single unitary Hermitian operator Ω . The Hamiltonian can be separated into two parts,

$$H = C_\Omega + A_\Omega, \quad (7)$$

with

$$C_\Omega \equiv (H + \Omega H \Omega)/2, \quad (8a)$$

$$A_\Omega \equiv (H - \Omega H \Omega)/2. \quad (8b)$$

Ω commutes with C_Ω and anti-commutes with A_Ω , i.e.,

$$\Omega C_\Omega \Omega = C_\Omega, \quad (9a)$$

$$\Omega A_\Omega \Omega = -A_\Omega. \quad (9b)$$

With an instantaneous control pulse Ω applied at the middle of the evolution time, the evolution operator becomes

$$\begin{aligned} U_\Omega(T) &= e^{-iHT/2} \Omega e^{-iHT/2} = \Omega e^{-i\Omega H \Omega T/2} e^{-iHT/2} \\ &= \Omega e^{-iC_\Omega T} + O(T^2), \end{aligned} \quad (10)$$

which commutes with Ω up to an error of $O(T^2)$. In general, one may apply an additional pulse at the end of evolution so that

$$[\Omega] U_0(T/2) \Omega U_0(T/2) \equiv e^{-iH_\Omega T}, \quad (11)$$

where $U_0(\tau) \equiv e^{-iH\tau}$ is the free evolution operator over time τ , and the brackets around the operation at the end of the sequence ($[\Omega]$) mean that the operation is optional. The effective Hamiltonian H_Ω commutes with Ω up to $O(T)$. Therefore Ω is protected to the first order.

Following the method given above, we can preserve more operators $\{\Omega_k\}$ in an MOOS by concatenation. The first level of control is

$$U_1(T) = [\Omega_1] U_0(T/2) \Omega_1 U_0(T/2) = e^{-iH_1 T}, \quad (12)$$

where the effective Hamiltonian H_1 commutes with Ω_1 up to $O(T)$. By treating the effective Hamiltonian as a new Hamiltonian on the second level, the propagator reads

$$U_2(T) = [\Omega_2] U_1(T/2) \Omega_2 U_1(T/2) = e^{-iH_2 T}, \quad (13)$$

where the effective Hamiltonian H_2 commutes with Ω_2 up to an error of $O(T)$. And according to Theorem 1, H_2 also commutes with Ω_1 up to $O(T)$. A general first order scheme is achieved by using Eq. (11) iteratively,

$$U_L(T) = [\Omega_L] U_{L-1}(T/2) \Omega_L U_{L-1}(T/2) = e^{-iH_L T}, \quad (14)$$

where the effective Hamiltonian H_L commutes with all operators in the MOOS $\{\Omega_i\}_{i=1}^L$ up to $O(T)$. Note that when the optional pulses are not used, only one pulse is applied at each time of operation.

It should be pointed out that the current DD scheme constructed by iteration is not the same as the symmetrization procedure described in Refs. [8] and [9]. For M -level systems, when $\log_2 M$ is not an integer, our scheme in general cannot achieve protection of all system operators. For example, when M is odd, our scheme can only protect operators diagonal in a certain basis. When $M = 2^L$, all system operators can be protected by protecting the MOOS of size $2L$. Several advantages of the MOOS-based DD, however, are worth mentioning. First, there are systematic ways to construct higher order DD for protecting all operators in an MOOS and hence the Lie algebra generated from the MOOS (Secs. II C and II D). Second, for multi-qubit systems, our scheme automatically gives DD sequences involving only single-qubit operations (Sec. III). Third, there is an explicit scheme to incorporate pulses of finite amplitude to DD (Sec. IV). Fourth, since the DD sequences on the inner levels use more control pulses than the sequences on the outer levels, qubits subjected to faster error sources can be protected on inner levels for economic use of control resources. For example, in a coupled electron-nuclear spin system, the electron spin, which has much faster decoherence than a nuclear spin does, should be controlled on the inner level.

C. Higher order protection by CDD

To go beyond the lowest order protection, let us consider a general sequence of unitary operations $\{\sigma_k\}$ on the system, where σ_k can be the identity operator. The evolution from $t = 0$ to T reads

$$U_C(T) = \sigma_{k_n}^\dagger e^{-iH(T-t_n)} \sigma_{k_n} \dots \sigma_{k_1}^\dagger e^{-iH(t_2-t_1)} \sigma_{k_1} \sigma_{k_0}^\dagger e^{-iHt_1} \sigma_{k_0} \\ \equiv \mathcal{T} \exp \left[-i \int_0^T H_\sigma(t) dt \right], \quad (15)$$

where \mathcal{T} is the time ordering operator, and $H_\sigma(t) \equiv \sigma_{k_j}^\dagger H \sigma_{k_j}$ for $t \in (t_j, t_{j+1}]$. In the standard time-dependent perturbation theory formalism, the propagator is expanded up to the second order as

$$U_C(T) = 1 + \sum_i h_i + \sum_{i>j} h_i h_j + \sum_i \frac{1}{2} h_i^2 + O(T^3), \quad (16)$$

where $h_j \equiv -i(t_{j+1} - t_j) H_\sigma(t)$ (with $t_0 \equiv 0$ and $t_{n+1} \equiv T$). In this paper we assume that this expansion converges, which means that the bath is bounded in spectrum.

It was shown that if $U_C(T)$ realizes the first order DD, i.e., $[\sum_{i=0}^n h_i, Q_j] = 0$ for a set of operators $\{Q_j\}$, then the second order DD can be realized by the symmetrized evolution [5, 9]

$$U_{\text{SDD}}(2T) \equiv \bar{U}_C U_C \\ = 1 + 2 \sum_{i=0}^n h_i + \frac{1}{2!} \left(2 \sum_{i=0}^n h_i \right)^2 + O(T^3), \quad (17)$$

where $\bar{U}_C \equiv e^{h_0} e^{h_1} \dots e^{h_{n-1}} e^{h_n}$ is mirror-symmetric with U_C .

For DD to even higher orders, in principle we can obtain the optimal sequences by solving Eq. (16) so that up to some order in the expansion, $U_C(T)$ commutes with a given set of operators. The third order terms read

$$\sum_{i>j>k} h_i h_j h_k + \sum_{i>j} \frac{1}{2!} h_i^2 h_j + \sum_{i>j} \frac{1}{2!} h_i h_j^2 + \sum_i \frac{1}{3!} h_i^3,$$

and in general $\sum_{j_1>j_2>\dots>j_n} h_{j_1}^{p_1} h_{j_2}^{p_2} \dots h_{j_n}^{p_n} \prod_{r=1}^n \frac{1}{p_r!}$ contains terms of the order $\sum_{r=1}^n p_r$. Finding solutions becomes formidable when the DD order is high.

If we are not concerned with the exponentially increasing number of control pulses, we can follow the idea of CDD [12, 14] to construct DD sequences in a systematic way to protect the operators $\{\Omega_l\}_{l=1}^L$ to an arbitrary DD order. The first order DD given by Eq. (14) is 2^L evolution operators $U(T/2^L)$ embedded in a sequence of control pulses $\{\Omega_l\}$. We denote this structure as

$$U_L^{[1]}(T) \equiv \Omega_L U_{L-1}(T/2) \Omega_L U_{L-1}(T/2) \\ \equiv C_\Omega \{U(T/2^L)\} = e^{-iH_L^{[1]}T}, \quad (18)$$

which is the first order CDD as defined in Eq. (14). The resultant first-order effective Hamiltonian $H_L^{[1]}$ commutes with the operators $\{\Omega_l\}_{l=1}^L$ up to an error of $O(T)$. Here the sequence $C_\Omega \{\dots\}$ makes the effective Hamiltonian commute

with $\{\Omega_l\}_{l=1}^L$ to a higher order. The evolution under the second order CDD

$$U_L^{[2]}(T) = C_\Omega \{U_L^{[1]}(T/2^L)\} = e^{-iH_L^{[2]}T}, \quad (19)$$

is obtained by replacing the free evolution $U(T/2^L)$ in Eq. (18) with $U_L^{[1]}(T/2^L)$, an evolution operator under the first order CDD control. The resultant effective Hamiltonian $H_L^{[2]}$ commutes with $\{\Omega_l\}_{l=1}^L$ up to an error of $O(T^2)$. Iteratively, the N th order CDD reads

$$U_L^{[N]}(T) = C_\Omega \{U_L^{[N-1]}(T/2^L)\}, \quad (20)$$

which preserves any operators in $\{\Omega_l\}_{l=1}^L$ up to $O(T^{N+1})$. Note that in the above construction of CDD, Theorem 1 has not been invoked, except in construction of the innermost level as in Eq. (14). The only requirement is that all the intervals of the outer level are equal so that the resultant effective Hamiltonian from the inner level of control is time-independent.

An alternative construction of CDD is given as follows. We first construct a CDD sequence to protect Ω_1 up to an error of $O(T^{N_1+1})$ by recursion

$$U_{\Omega_1}^{C[N_1]}(T) = \Omega_1 U_{\Omega_1}^{C[N_1-1]}(T/2) \Omega_1 U_{\Omega_1}^{C[N_1-1]}(T/2), \quad (21)$$

with $U_{\Omega_1}^{C[0]}(T) \equiv U(T)$ and the superscript C denoting the nesting scheme of CDD. By defining $U_{\Omega_1, \Omega_2}^{C[N_1, 0]}(T) \equiv U_{\Omega_1}^{C[N_1]}(T)$, we can construct a further level of CDD to protect Ω_2 up to $O(T^{N_2+1})$, by the recursion

$$U_{\Omega_1, \Omega_2}^{C[N_1, N_2]}(T) = \Omega_2 U_{\Omega_1, \Omega_2}^{C[N_1, N_2-1]}(T/2) \Omega_2 U_{\Omega_1, \Omega_2}^{C[N_1, N_2-1]}(T/2). \quad (22)$$

Similarly, we have the propagator by recursion

$$U_{\Omega_1, \Omega_2, \dots, \Omega_{l-1}, \Omega_l}^{C[N_1, N_2, \dots, N_l, 0]}(T) \equiv U_{\Omega_1, \Omega_2, \dots, \Omega_l}^{C[N_1, N_2, \dots, N_l]}(T), \quad (23a)$$

$$U_{\Omega_1, \Omega_2, \dots, \Omega_L}^{C[N_1, \dots, N_L]}(T) = \Omega_L U_{\Omega_1, \Omega_2, \dots, \Omega_L}^{C[N_1, \dots, N_L-1]}(T/2) \Omega_L \\ \times U_{\Omega_1, \Omega_2, \dots, \Omega_L}^{C[N_1, \dots, N_L-1]}(T/2). \quad (23b)$$

According to Theorem 1, the inner levels of DD are unaffected by the outer levels of control. Thus the evolution $U_{\Omega_1, \Omega_2, \dots, \Omega_L}^{C[N_1, N_2, \dots, N_L]}(T)$ commutes with $\Omega_1, \Omega_2, \dots, \Omega_L$ to the orders N_1, N_2, \dots, N_L , in turn. An advantage of this construction is that the errors induced by Ω_l are eliminated independently and to different orders $\{N_l\}$, which allows protecting operators with stronger error sources to higher orders. For example, usually for spin qubits under strong external magnetic field, the pure dephasing is much faster than the population relaxation, so it is favorable to protect the phase correlation on the inner level and to a higher CDD order.

The number of operations required in preserving the operators is $\sim 2^{N_L}$ for the CDD scheme in Eq. (20) or $\sim 2^{\sum_{l=1}^L N_l}$ for that in Eq. (23). They increase exponentially with the DD order. Even though the exponentially increasing number of control pulses does yield significant improvement of precision (through reduction of the coefficient in front of the power of time T^{N+1}) [11, 35, 36], implementation of CDD to high orders is challenging in experiments since errors are inevitably introduced in each control pulse.

D. Higher order protection by NUDD

If there is only one unitary Hermitian operator Ω to be preserved, N operations of Ω applied at the UDD timing [16]

$$T_n = T \sin^2 \frac{n\pi}{2N+2}, \text{ for } n = 1, \dots, N, \quad (24)$$

during the evolution from $T_0 \equiv 0$ to $T_{N+1} \equiv T$ protect the physical quantity Ω to the N th order [37]. Explicitly, the propagator under control

$$U_\Omega^{[N]}(T) \equiv \Omega^N U_0(\tau_N) \cdots \Omega U_0(\tau_1) \Omega U_0(\tau_0), \quad (25)$$

commutes with Ω up to an error of $O(T^{N+1})$. Here the evolution intervals are

$$\tau_n \equiv T_{n+1} - T_n = \frac{T}{2} \left[\cos \frac{n\pi}{N+1} - \cos \frac{(n+1)\pi}{N+1} \right]. \quad (26)$$

When there are more than one unitary Hermitian operators $\{\Omega_i\}_{i=1}^L$ to be protected, the question is whether we can construct NUDD so that the number of control pulses scales polynomially with the protection order. A known example is QDD, in which UDD of, e.g., σ_z and σ_x are nested. For general cases, we establish the following theorem as the basis of NUDD.

1. A theorem on UDD control of time-dependent systems

Theorem 2. *For a finite-norm time-dependent Hamiltonian $H(t)$ defined in $[0, T]$, an N th order UDD control with N operations of unitary Hermitian operator Ω applied at T_1, T_2, \dots, T_N preserves Ω up to an error of $O(T^{N+1})$, if*

$$H(T_n + s\tau_n) = H(T_{n+1} - s\tau_n) = H(sT_1), \quad (27)$$

for $s \in [0, 1]$ and $\tau_n = T_{n+1} - T_n$, i.e., the Hamiltonian has the same form as a function of the relative time between adjacent operations and is symmetric within each interval.

Note: The previous extension of UDD to time-dependent systems requires that the Hamiltonians be analytic (having smooth time-dependence) [27, 29, 37]. In Theorem 2, the Hamiltonians are not required to be analytic but with certain symmetries. The symmetry requirements on the time-dependence of the Hamiltonians can actually be fulfilled by designing the timing of DD sequences on the inner levels so that recursive nesting of DD is possible.

Proof. The evolution under the control of Ω reads

$$U(T) = \Omega^N V_N \Omega V_{N-1} \cdots \Omega V_1 \Omega V_0, \quad (28)$$

with the evolution operator

$$\begin{aligned} V_n &\equiv \mathcal{T} \exp \left[-i \int_{T_n}^{T_{n+1}} H(t) dt \right] \\ &\equiv \mathcal{T}_\theta \exp \left[-i \tau_n \int_{\frac{n}{N+1}\pi}^{\frac{n+1}{N+1}\pi} H^{\text{rel}}(\theta) d\theta \right], \end{aligned} \quad (29)$$

where \mathcal{T}_θ stands for ordering in θ , and

$$H^{\text{rel}}(\theta) = \frac{N+1}{\pi} H(t), \quad (30)$$

where $\theta = \frac{n\pi}{N+1} + \frac{t-T_n}{\tau_n} \frac{\pi}{N+1}$ for $t \in (T_n, T_{n+1}]$. The symmetry requirements given in Eq. (27) are transformed to

$$H^{\text{rel}}\left(\frac{n\pi}{N+1} + \theta\right) = H^{\text{rel}}\left(\frac{n+1}{N+1}\pi - \theta\right) = H^{\text{rel}}(\theta). \quad (31)$$

The Hamiltonian $H^{\text{rel}}(\theta)$ can be separated into two parts,

$$H^{\text{rel}}(\theta) = C(\theta) + A(\theta), \quad (32)$$

with

$$C(\theta) = [H^{\text{rel}}(\theta) + \Omega H^{\text{rel}}(\theta) \Omega] / 2, \quad (33a)$$

$$A(\theta) = [H^{\text{rel}}(\theta) - \Omega H^{\text{rel}}(\theta) \Omega] / 2. \quad (33b)$$

$C(\theta)$ and $A(\theta)$ commute and anti-commute with the operator Ω , respectively.

Now we rewrite the propagator as

$$U(T) = \mathcal{T}_\theta \exp \left[-iT \int_0^\pi G(\theta) (C(\theta) + F(\theta) A(\theta)) d\theta \right], \quad (34)$$

where

$$G(\theta) = \frac{1}{2} \left[\cos \frac{n\pi}{N+1} - \cos \frac{(n+1)\pi}{N+1} \right], \quad (35a)$$

$$F(\theta) = (-1)^n, \quad (35b)$$

for $\theta \in \left(\frac{n\pi}{N+1}, \frac{(n+1)\pi}{N+1} \right]$. Thus, the part of Hamiltonian $C(\theta)$ that commutes with Ω is modulated by the step function $G(\theta)$ which has step heights given by the UDD intervals, and the part of Hamiltonian $A(\theta)$ that anti-commutes with Ω is modulated by $G(\theta)$ and the periodic modulation function $F(\theta)$. Furthermore, both $C(\theta)$ and $A(\theta)$ have the same symmetries as $H^{\text{rel}}(\theta)$ in Eq. (31). The symmetries of the time-dependent Hamiltonian and the modulation functions make them have particular Fourier expansions, which lead us to a proof of the theorem in a procedure similar to the proof of UDD in Ref. [19].

The Fourier expansions of the modulation functions and the time-dependent Hamiltonians are

$$G(\theta) = \sum_{k=0}^{\infty} g_k \sin[2k(N+1)\theta \pm \theta], \quad (36a)$$

$$F(\theta) = \sum_{k=0}^{\infty} f_k \sin[(2k+1)(N+1)\theta], \quad (36b)$$

$$C(\theta) = \sum_{k=0}^{\infty} c_k \cos[2k(N+1)\theta], \quad (36c)$$

$$A(\theta) = \sum_{k=0}^{\infty} a_k \cos[2k(N+1)\theta]. \quad (36d)$$

Here the operators c_k and a_k commute and anti-commute with Ω , respectively. The features of these Fourier expansions to

be used in the proof below are: (i) Both C and A contain only cosine harmonics of order of even multiple of $(N + 1)$; (ii) $F(\theta)$ contains only sine harmonics of order of odd multiple of $(N + 1)$; $G(\theta)$ contains only sine harmonics of an order differing from an even multiple of $(N + 1)$ by $+1$ or -1 .

With the product-to-sum trigonometric formulae, we have

$$U(T) = \mathcal{T}_\theta \exp \left[-iT \int_0^\pi (\tilde{C}(\theta) + \tilde{A}(\theta)) d\theta \right], \quad (37)$$

with

$$\tilde{C}(\theta) \equiv G(\theta)C(\theta) = \sum_k \tilde{c}_k \sin[2k(N + 1)\theta \pm \theta], \quad (38a)$$

$$\begin{aligned} \tilde{A}(\theta) &\equiv G(\theta)F(\theta)A(\theta) \\ &= \sum_k \tilde{a}_k \cos[(2k + 1)(N + 1)\theta \pm \theta]. \end{aligned} \quad (38b)$$

A straightforward method is to expand $U(T)$ according to the standard time-dependent perturbation theory. It should be noted that such perturbation-theoretic expansion requires that the modulated Hamiltonian have bounded norm. In the expansion, the terms which do not commute with Ω must contain an odd times of $\{\tilde{a}_k\}$ (since Ω anti-commutes with $\{\tilde{a}_k\}$). The expansion coefficients can be written as

$$\begin{aligned} &(-iT)^n \times \\ &\int_0^\pi y_{k_1}^{\alpha_1, \eta_1}(\theta_1) \int_0^{\theta_1} y_{k_2}^{\alpha_2, \eta_2}(\theta_2) \cdots \int_0^{\theta_{n-1}} y_{k_n}^{\alpha_n, \eta_n}(\theta_n) d\theta_1 \cdots d\theta_n, \end{aligned} \quad (39)$$

with $y_k^{s,\pm}(\theta) \equiv \sin[2k(N + 1)\theta \pm \theta]$ associated with an operator \tilde{c}_k , and $y_k^{c,\pm}(\theta) \equiv \cos[(2k + 1)(N + 1)\theta \pm \theta]$ associated with an operator \tilde{a}_k , for $\alpha_j \in \{c, s\}$ and $\eta_j \in \{+, -\}$. By induction and repeatedly using the product-to-sum trigonometric formulae, one can straightforwardly verify that the coefficients in Eq. (39) vanish for $n \leq N$ and $y_k^{c,\pm}$ appearing an odd number of times. Thus vanish any terms in the expansion which contain products of an odd number of operators in $\{\tilde{a}_k\}$ and have a power of T lower than $(N + 1)$. \square

2. NUDD

For a time-independent Hamiltonian H under DD control of instantaneous operations of a unitary Hermitian operator Ω applied at $t_1, t_2, \dots, t_{N'}$, the evolution $U(\tau)$ from $t_0 = 0$ to $t_{N'+1} = \tau$ is equivalent to the evolution under a time-dependent Hamiltonian

$$H(t) = \Omega^n H \Omega^n, \quad (40)$$

for $t \in (t_n, t_{n+1}]$. Such time-dependence is not analytic. If N' is an even number and the operation sequence is symmetric, the time-dependent Hamiltonian $H(t)$ is time symmetric in $[0, \tau]$. Thus, according to Theorem 2, in a UDD sequence of an operator Ω applied at T_1, T_2, \dots, T_N between $T_0 = 0$

and $T_{N+1} = T$, each interval of free evolution $e^{-iH(T_{n+1}-T_n)}$ can be substituted with the evolution inserted by a sequence of another operation Ω' applied at $T_{n,1}, T_{n,2}, \dots, T_{n,N'}$ between $T_{n,0} \equiv T_n$ and $T_{n,(N'+1)} \equiv T_{n+1}$, with the same symmetric structure in all intervals, i.e.,

$$T_{n+1} - T_{n,N'-k} = T_{n,k+1} - T_n, \quad (41a)$$

$$\frac{T_{n,k} - T_{n,k'}}{T_{n+1} - T_n} = \frac{T_{m,k} - T_{m,k'}}{T_{m+1} - T_m}. \quad (41b)$$

In particular, the inner level control of Ω' can be chosen as an even order UDD.

Now we describe the construction of NUDD for protecting a set of unitary Hermitian operators $\{\Omega_l\}_{l=1}^L$. First, the N_L th order UDD sequence of Ω_L is constructed with pulses applied at

$$T_{n_L} = T \sin^2 \frac{n_L \pi}{2N_L + 2}, \quad (42)$$

between $T_0 = 0$ and $T_{N_L+1} = T$ as the outermost level of control. N_L could be either odd or even. Then the free evolution in each interval is substituted by the N_{L-1} th order UDD sequence of Ω_{L-1} applied at

$$T_{n_L, n_{L-1}} = T_{n_L} + (T_{n_L+1} - T_{n_L}) \sin^2 \frac{n_{L-1} \pi}{2N_{L-1} + 2}, \quad (43)$$

in each interval between $T_{n_L,0} \equiv T_{n_L}$ and $T_{n_L, N_{L-1}+1} \equiv T_{n_L+1}$, with N_{L-1} being an *even* number. So on and so forth, the l th level of control is constructed by applying N_l times of Ω_l in each interval between $T_{n_L, \dots, n_{l+1},0} \equiv T_{n_L, \dots, n_{l+2}, n_{l+1}}$ and $T_{n_L, \dots, n_{l+1}, N_l+1} \equiv T_{n_L, \dots, n_{l+2}, n_{l+1}+1}$ at

$$\begin{aligned} T_{n_L, \dots, n_{l+1}, n_l} &= T_{n_L, \dots, n_{l+1}} \\ &+ [T_{n_L, \dots, n_{l+2}, n_{l+1}+1} - T_{n_L, \dots, n_{l+1}}] \sin^2 \frac{n_l \pi}{2N_l + 2}, \end{aligned} \quad (44)$$

with N_l being an *even* number. We denote the evolution under such NUDD as $U_{\Omega_1, \Omega_2, \dots, \Omega_L}^{U[N_1, N_2, \dots, N_L]}(T)$, where the superscript U denotes the nesting of UDD sequences.

According to Theorem 2, the outer levels of UDD control are not affected by the inner levels of even-order UDD control. And according to Theorem 1, the inner levels of DD control are not affect by the outer levels of control since $\{\Omega_l\}$ is an MOOS. Thus each operator Ω_l is protected up to an error of $O(T^{N_l+1})$. The number of control intervals is

$$N_{\text{pulse}}^{U[N_1, N_2, \dots, N_L]} = (N_1 + 1)(N_2 + 1) \cdots (N_L + 1), \quad (45)$$

increasing polynomially with the decoupling order.

III. NUDD OF MULTI-QUBIT SYSTEMS

A. General multi-qubit systems

To protect a multi-qubit system to a given order of precision, we just need to protect the operators in an MOOS described in Sec. II A, by using the method depicted in Sec. II B

for the first order preservation, or by using the NUDD scheme in Sec. IID for higher order preservation. Since for general multi-qubit systems, the MOOS can be chosen as a set of single-qubit operators such as the Pauli matrices $\{\sigma_x^{(l)}, \sigma_z^{(l)}\}_{l=1}^L$, NUDD can be implemented with only single-qubit flips.

In suppressing the relaxation or pure dephasing to the first order, i.e., in protecting the MOOS $\{\sigma_z^{(l)}\}_{l=1}^L$ or $\{\sigma_x^{(l)}\}_{l=1}^L$, the first order scheme in Sec. IIB requires 2^L pulse intervals. For suppressing decoherence in general cases, the first order scheme requires 4^L intervals to protect the MOOS $\{\sigma_x^{(l)}, \sigma_z^{(l)}\}_{l=1}^L$. Such numbers of intervals are actually the minima required for protecting L -qubit systems, as proven in Ref. [31]. In preserving the coherence of a multi-qubit system to an arbitrarily high order of precision by NUDD, the number of intervals given in Eq. (45) increases polynomially with the decoupling orders, much less than that required in CDD. A question is whether NUDD is optimal or nearly optimal in terms of the number of control pulses. For QDD control of one qubit, numerical check up to the fourth order indicates that NUDD is nearly optimal, differing from the optimal solutions by less than 3 control pulses [26]. NUDD of a larger MOOS, however, can be shown to be far from the optimal in the second decoupling order: For an L -qubit system suffering pure dephasing, an L -level NUDD in the second order requires $\sim 3^L$ control intervals, while the SDD, which uses two mutually symmetric first order DD sequences to realize the second order control (see Sec. IIC), requires only 2×2^L intervals. We expect that in higher orders of DD, there exist DD schemes (using only single-qubit control for multi-qubit systems) much more efficient than NUDD. But no explicit solutions are known to us, except for a few numerical solutions.

B. Discussions on QDD

In particular, for a single-qubit system, NUDD reduces to QDD with even order DD on the inner level. Explicitly the nested sequence $U_{\sigma_z, \sigma_x}^{U[2N_1, N_2]}(T)$ is the QDD sequence protecting the MOOS operators σ_z and σ_x to orders $2N_1$ and N_2 , respectively. Thus based on Theorems 1 and 2, the validity of QDD with even order UDD on the inner level is proven.

But Theorem 2 does not apply to the case of odd order UDD control on the inner level. Actually, when the inner level UDD has an odd order, which breaks the symmetry condition of the theorem, the outer level UDD may be spoiled. For a specific example, let us consider the control of a Hamiltonian like

$$H = J_0 + J_1\Omega_1 + J_2\Omega_2 + J_{1,2}\Omega_1\Omega_2,$$

where J_0, J_1, J_2 , and $J_{1,2}$ are arbitrary bath operators, and Ω_1 and Ω_2 are two system operators forming an MOOS (such as $\Omega_1 = \sigma_z$ and $\Omega_2 = \sigma_x$ for a single-qubit system). We choose the inner level control as the first order UDD of Ω_1 and the outer level as the second order UDD of Ω_2 . The propagator of this NUDD is

$$U_{\Omega_1, \Omega_2}^{U[1,2]}(T) = (\Omega_1 e^{-iH\tau} \Omega_1 e^{-iH\tau}) \Omega_2 (\Omega_1 e^{-iH2\tau} \Omega_1 e^{-iH2\tau}) \Omega_2 \\ \times (\Omega_1 e^{-iH\tau} \Omega_1 e^{-iH\tau}), \quad (46)$$

where the evolution in each pair of parentheses corresponds to the UDD control on the inner level and $\tau = T/8$. The time expansion gives

$$U_{\Omega_1, \Omega_2}^{U[1,2]}(T) = U_B + \Omega_1 O(T^2) + \Omega_1 \Omega_2 O(T^2) + O(T^3), \quad (47)$$

where U_B is a pure bath evolution operator. Thus even though a second order UDD sequence of Ω_2 is applied, Ω_2 is preserved only to the first order.

The above example indicates that the effective Hamiltonian resulting from the inner level UDD control can not be written into an analytic form. Otherwise, according to Ref. [27], which establishes the performance of UDD on analytically time-dependent systems, the outer level UDD should not be affected. As proposed in Ref. [27], for an NUDD evolution

$$U_{\Omega_1, \Omega_2}^{U[N', N]}(T) = \Omega_2^N U_{\Omega_1}^{U[N']}(T_N) \Omega_2 \cdots U_{\Omega_1}^{U[N']}(T_1) \Omega_2 U_{\Omega_1}^{U[N']}(T_0),$$

one can define the effective Hamiltonian resulting from the inner level of control as

$$\tilde{H}_{\text{eff}}(T_n + t) \equiv i \left[\partial_t U_{\Omega_1}^{U[N']}(t) \right] \left[U_{\Omega_1}^{U[N']}(t) \right]^\dagger, \quad (48)$$

for $t \in (0, \tau_n]$. The outer level UDD can be viewed as acting on this effective Hamiltonian. The Hamiltonian defined in Eq. (48), however, is only piecewise analytic and is even discontinuous at T_n 's. Therefore, the theorem established in Ref. [27] about UDD control of analytically time-dependent systems does not apply to QDD.

Thus, the complete proof (or disproof) of the validation of QDD is still an open question. We should mention that if QDD is proven valid for one qubit, according to our formalism of nested DD, the same NUDD is also valid for any two operators forming an MOOS. In this way the QDD control can be generalized, in particular, to the protection of two-qubit systems from dephasing and disentanglement, etc.

IV. DD BY PULSES OF FINITE AMPLITUDE

The ideal instantaneous pulses are not realistic in experiments since they would contain an infinite amount of energy. Of course, when the pulses are much shorter than the other timescales of the system and the bath, it is a good approximation to treat them as infinitely short. But if this condition is not satisfied, it is of interest to consider DD by pulses of finite amplitude. The problem of first order DD with finite-amplitude pulses has been considered within the Eulerian DD framework [38] and in a geometric picture [39]. It is possible to achieve arbitrary control precision by recursive construction of pulse shapes [40]. DD of single-qubit systems using finite-amplitude pulses up to a control error in the second order of pulse durations has been presented in Refs. [32, 41]. In UDD, finite-amplitude pulses of higher orders of control precision can also be incorporated [20].

Here we consider the general case of DD by finite-amplitude pulses. Let us consider a short-pulse operation by the Hamiltonian

$$H_\Omega(t) = v(t)\Omega, \quad (49)$$

where Ω is a unitary Hermitian operator. We aim to design the pulse shape of $v(t)$ such that the evolution during the pulse control approximates the ideal δ -pulse control up to a certain order of the pulse duration τ_p , i.e.,

$$U(\tau_p, 0) = \mathcal{T} \exp \left[-i \int_0^{\tau_p} [H + H_\Omega(t)] dt \right] = e^{-i(\tau_p - \tau_s)H} P_\Omega e^{-i\tau_s H} + O(\tau_p^{M_p}), \quad (50)$$

where $P_\Omega \equiv \exp \left[-i \int_0^{\tau_p} H_\Omega(t) dt \right]$ is the desired instantaneous control applied at the time τ_s . In particular, we need the π pulse $P_\Omega = \Omega$ up to a trivial global phase factor. Unfortunately, a no-go theorem established in Ref. [32, 41] restricts that instantaneous π pulses can not be approximated by a finite-amplitude pulse with error lower than $O(\tau_p^2)$ without perturbing the bath evolution. Thus, here we focus on the first order pulse shaping with $M_p = 2$.

We write the evolution operator as

$$U(\tau_p, 0) = e^{-i(\tau_p - \tau_s)H} U_\Omega e^{-i\tau_s H}, \quad (51)$$

where

$$U_\Omega = \mathcal{T} \exp \left[-i \int_0^{\tau_p} \tilde{H}_\Omega(t) dt \right], \quad (52)$$

with $\tilde{H}_\Omega(t) \equiv e^{iH(t-\tau_s)} H_\Omega(t) e^{-iH(t-\tau_s)}$. The correction term is

$$\begin{aligned} h_\Omega(t) &\equiv \tilde{H}_\Omega(t) - H_\Omega(t) \\ &= v(t) \sum_{k=1}^{\infty} \frac{(t - \tau_s)^k}{k!} \underbrace{[iH, [iH, \dots [iH, \Omega] \dots]]}_{k \text{ folds}}. \end{aligned} \quad (53)$$

We want to design $v(t)$ such that the control error

$$\begin{aligned} \delta P_\Omega &\equiv U_\Omega - P_\Omega \\ &= \mathcal{T} \left\{ e^{-i \int_0^{\tau_p} H_\Omega(t) dt} \left[e^{-i \int_0^{\tau_p} h_\Omega(t) dt} - 1 \right] \right\} = O(\tau_p^2). \end{aligned} \quad (54)$$

The leading order term in δP_Ω is

$$\begin{aligned} \eta^{(1)} &= \mathcal{T} \left\{ e^{-i \int_0^{\tau_p} H_\Omega(t) dt} \int_0^{\tau_p} (t - \tau_s) v(t) [H, \Omega] dt \right\} \\ &= \int_0^{\tau_p} (t - \tau_s) v(t) e^{-i \int_t^{\tau_p} H_\Omega(s) ds} [H, \Omega] e^{-i \int_0^t H_\Omega(s) ds} dt. \end{aligned} \quad (55)$$

Using $\Omega^2 = 1$ and $H_\Omega(t) = v(t)\Omega$, we have

$$e^{-i \int_{t_1}^{t_2} H_\Omega(s) ds} = \cos \left[\int_{t_1}^{t_2} v(s) ds \right] - i\Omega \sin \left[\int_{t_1}^{t_2} v(s) ds \right]. \quad (56)$$

Now we decompose the Hamiltonian H into two parts as $H = A + C$, with A and C anti-commuting and commuting with Ω , respectively. The leading order error term in Eq. (55) becomes

$$\eta^{(1)} = [A, \Omega] \eta_{11} - i\Omega [A, \Omega] \eta_{12}, \quad (57)$$

where

$$\eta_{11} = \int_0^{\tau_p} (t - \tau_s) v(t) \cos [\phi_0 - \psi(t)] dt, \quad (58a)$$

$$\eta_{12} = \int_0^{\tau_p} (t - \tau_s) v(t) \sin [\phi_0 - \psi(t)] dt, \quad (58b)$$

with $\psi(t) \equiv 2 \int_{\tau_s}^t v(s) ds$ and $\phi_0 = \int_{\tau_s}^{\tau_p} v(s) ds - \int_0^{\tau_s} v(s) ds$. To eliminate the leading order error, we just need to make $\eta_{11} = \eta_{12} = 0$, which are the same as those derived in Ref. [32] for single-qubit flip control.

Using the finite-amplitude pulses designed as depicted above, we can realize DD based on an MOOS up to an error in the second order of the pulse duration. Note that in some DD schemes, such as CDD $U_{\Omega_1, \dots, \Omega_L}^{C[N_1, \dots, N_L]}(T)$ as shown in Eq. (23), operations of different Ω_i 's may coincide. For example, Ω_1 , Ω_2 , and Ω_3 coincide at the end of the sequence $U_{\Omega_1, \Omega_2, \Omega_3}^{C[N_1, N_2, N_3]}(T)$. In this case, we can define a new unitary Hermitian operator Ω' as the product of the operations (such as $\Omega_1 \Omega_2 \Omega_3$ in the example), and design the pulse $H_{\Omega'}(t) = v(t)\Omega'$ to achieve the operation up to an error of $O(\tau_p^2)$. Such finite-amplitude pulse operation, however, would involve multi-qubit interactions and may not be easy to be implemented in experiments, unless Ω' happens to be a single-qubit operation. This problem, fortunately, does not exist in NUDD, since there no two operations coincide, which stands for another advantage of NUDD over CDD.

Ref. [20] has presented a method to implement UDD by higher order shaped pulses. At the first sight, it seems that those pulses can be incorporated in NUDD. However, the method in Ref. [20] requires a starting and a stopping pulse to protect the UDD sequence. In NUDD, such starting and stopping operations will be mixed up with the outer level control applied at the same time. Then the operations on the outer levels need to be redesigned, which may be much more complicated than the design in Ref. [20] since different operations may interfere with each other and multi-qubit interactions may be involved. Explicit implementation of NUDD with finite-amplitude pulses of higher order control accuracy is an interesting topic for future work.

V. CONCLUSIONS AND DISCUSSIONS

Based on two theorems, we have presented explicit schemes of dynamical decoupling to preserve operators in an MOOS (i.e., unitary Hermitian operators which either commute or anti-commute with each other) to arbitrary decoupling orders for quantum systems arbitrarily coupled to quantum baths. All system operators in a Lie algebra generated from the MOOS by commutation, anti-commutation, linear combinations, and repetitions are also preserved. Theorem 1 states that the inner levels of DD control are unaffected by the outer levels if the control operations are elements of an MOOS. Theorem 2 states that UDD still works if the Hamiltonians in different intervals have the same function form of the relative time and are symmetric, regardless of the analytic properties of the Hamiltonians. These theorems enable a construction of higher order DD by nesting UDD sequences of even orders. NUDD protects system operators in a Lie algebra generated from an MOOS to an arbitrary order of precision. For multi-qubit systems, any physical quantities can be protected, and NUDD can be implemented by single-qubit operations. For single-qubit systems, NUDD reduces to QDD with even order UDD on the inner level. Thus the theorems provide a rigorous

proof of the validity of QDD with even order DD on the inner level.

NUDD achieves a desired decoupling order with only a polynomial increase in the number of pulses, with exponential saving of the number of pulses as compared with CDD of the same decoupling order. In suppressing the general decoherence, the number of pulses still scales exponentially with the number of qubits. Such exponential increase, indeed, is required by a theorem which sets the minimum number of control intervals to be 4^L or 2^L for protecting a general or pure dephasing L -qubit system to the first decoupling order, respectively [31].

For Hamiltonians of certain structures, such as the Hamiltonians of qudit systems with bipartite interactions, reduction in the number of pulses is possible [42]. Fewer levels of nesting are required if the structures of the Hamiltonians are exploited and a proper MOOS is designed. The number of pulses can also be greatly reduced if we protect only some logically encoded qubits or some particular states of the system [28, 29, 43, 44]. For example, if we choose the MOOS as $\{\sigma_x^{(1)} \otimes \sigma_x^{(2)}, \sigma_z^{(1)}, \sigma_z^{(2)}\}$ for a two-qubit system, the only possible noise generator [38] after protection is $\sigma_z^{(1)} \otimes \sigma_z^{(2)}$, which commutes with all the elements in the MOOS; in this case, the logical qubit $\alpha|\uparrow\uparrow\rangle + \beta|\downarrow\downarrow\rangle$ or $\alpha'|\uparrow\downarrow\rangle + \beta'|\downarrow\uparrow\rangle$ is protected

by only three levels of nesting.

NUDD protecting two operators forming an MOOS is near-optimal and has the same timing as QDD. In general, however, NUDD is by far not optimal, since a large nesting level L requires much more control intervals than the symmetrized DD for achieving the second decoupling order. An interesting question for future study is how to construct optimal or nearly optimal higher-order DD for general multi-qubit or multi-level systems.

For realistic implementation of DD, we have derived the conditions for finite-amplitude pulses to simulate ideal operations up to an error in the second order of pulse duration, and the conditions reach the same results as for single-qubit flip control given in Ref. [32]. Thus we can apply the pulses designed in Ref. [32] to the higher order DD schemes for general quantum systems.

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